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iTOUGH2: FROM PARAMETER ESTIMATION TO MODEL STRUCTURE IDENTIFICATION

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ABSTRACT

iTOUGH2 provides inverse modeling capabilities for the TOUGH2 family of nonisothermal multiphase flow simulators. It can be used for a formalized sensitivity analysis, parameter estimation by automatic model calibration, and uncertainty propagation analyses. While iTOUGH2 has been successfully applied for the estimation of a variety of parameters based on different data types, it is recognized that errors in the conceptual model have a great impact on both the estimated parameters and the subsequent model predictions. Identification of the most suitable model structure is therefore one of the most important and most difficult tasks. Within the iTOUGH2 framework, model identification can be partly addressed through appropriate parameterization of alternative conceptual-model elements. In addition, statistical measures are provided that help rank the performance of different conceptual models. We present a number of features added to the code that allow for a better parameterization of conceptual model elements, specifically heterogeneity. We discuss how these new features can be used to support the identification of key model structure elements and their impact on model predictions.

INTRODUCTION

Numerical models such as TOUGH2 (Pruess et al., 1999) support a variety of scientific and engineering tasks, including the study of fundamental physical processes, the design, optimization, and analysis of laboratory and field experiments, and the prediction of the system behavior under natural conditions or in response to groundwater management decisions. Regardless of the purpose or application, modeling involves (1) conceptualizing the salient features of the hydrogeologic system of interest, (2) characterizing these features by means of a finite number of input parameters, and (3) solving the system of governing equations, which brings together the fundamental physical laws with problem-specific attributes for the estimation of the unknown system states.

Each of the modeling steps outlined above is associated with uncertainties as well as random and systematic errors. The generally high accuracy of TOUGH2 simulations has been frequently demonstrated (see, e.g., Moridis and Pruess, 1992), and continuous improvements are being made to increase the robustness of the numerical solution.

Modeling results may be strongly affected by incomplete knowledge about the numerous input parameters. These parameters are usually difficult to determine in the laboratory or the field. Moreover, they may be process- and scale-dependent, i.e., the "measured" parameters are often conceptually and thus numerically different from the effective parameters required by and most suitable for use in the site-specific numerical model.

Finally, an inappropriate simplification or error in the conceptual model is likely to have a significant impact on the simulations and the conclusions drawn from the modeling study. In summary, the conceptual model must be thoroughly examined and its parameters must be carefully determined to assess the reliability of otherwise accurate numerical predictions.

The inverse modeling code iTOUGH2 (Finsterle, 1999a, b, c) essentially examines the impact of input parameters on selected model outputs, and uses this information for automatic model calibration and uncertainty propagation analyses. This general framework could be expanded to also investigate alternative conceptual models, provided that the relevant aspects of the model structure can be suitably parameterized.

The combination of simulation and optimization techniques as implemented in iTOUGH2 is presented first, followed by a number of illustrative examples, which demonstrate the usefulness and limitations of automatic parameter estimation and model identification.

OPTIMIZATION FRAMEWORK

As discussed in the introduction, iTOUGH2 combines the simulation capabilities of TOUGH2 with optimization techniques to perform model calibration (inverse modeling), to support the design of experimental layouts, and to optimize remediation strategies. In all these application modes, a performance measure (also referred to as objective function) is either minimized or maximized by adjusting certain input parameters or design variables. For example, model calibration consists of reducing the differences between the simulation results and measured data (such as pressures, flow rates, concentrations, or temperatures) by adjusting the model input parameters (such as the absolute permeability, capillary strength, thermal conductivity or recharge rate). A cleanup operation can be improved by minimizing, for example, the remediation time, which can be achieved by increasing pumping rates or the temperature of the steam injected to vaporize volatile organic compounds. Increasing these operational parameters, however, leads to higher energy costs. Therefore, the objective function to be minimized should reflect both costs and benefits in order to obtain an optimal remediation design (for details, see Finsterle, 2000a).

In general, the objective function has the following form:

$$S = \sum_{i=1}^{m} \omega(y_i; \mathbf{p}) \tag{1}$$

where ω is an arbitrary loss function (usually the square or absolute value; for additional options, see Finsterle and Najita, 1998), and y_i is an appropriately weighted residual:

$$y_i = \frac{z_i^* - z_i(\mathbf{p})}{\sigma_i} \tag{2}$$

where z_i^* is one of m actual data points (or fictitious design values such as zero cost) at a discrete point i in space and/or time, and z_i is the corresponding TOUGH2 output variable, which is a function of the input parameter vector **p**. The weighting coefficient σ_i is often related to the measurement error. A number of algorithms are available in iTOUGH2 to minimize the objective function.

PARAMETERIZATION

TOUGH2 modeling (and modeling in general) is concerned with a simplified, abstracted, and parameterized representation of the natural system. While maintaining the salient features of the hydrogeologic system, some of its aspects and processes are lumped together and described by effective and/or averaged parameters. Model conceptualization and parameterization are therefore related, both trying to capture and reduce the essentially infinite complexity of the natural system. For example, complex molecular and pore-scale flow and transport processes are formulated based on a continuum approach, which results in effective parameters such as permeability and dispersivity. Moreover, heterogeneity in subsurface properties is approximated by average values assigned to each gridblock of the discretized model. Multiple gridblocks may be grouped together—a process referred to as “zonation.” Heterogeneity may also be described by geostatistical methods, in which spatial variability is characterized by a relatively small number of geostatistical parameters (such as variogram parameters, conditioning values at pilot points, attractor parameters).

As long as a feature or process is suitably parameterized, it can be subjected to estimation, optimization, sensitivity, and uncertainty analyses supported by iTOUGH2. Parameterization may not only include hydrogeologic properties (such as the heterogeneous permeability field), but also aspects of the conceptual model that are considered uncertain. For example, uncertainty in the initial conditions or boundary infiltration rate can be parameterized and estimated along with hydrogeologic properties. Moreover, a potential systematic error (such as a suspected drift in the data or leakage in a measurement device) can also be parameterized and included in the estimation or uncertainty analysis. An example of the latter is discussed in detail in Finsterle and Persoff (1997).

Sensitivity and uncertainty propagation analyses may involve as many parameters as desired. For inverse modeling purposes, however, it is often not sensible to estimate a large number of strongly correlated parameters based on limited data of insufficient sensitivity. Adding more parameters to vector **p** always leads to an improvement of the fit. However, if too many parameters are estimated simultaneously, the better reproduction of data comes at the expense of increased estimation uncertainty and thus reduced accuracy of subsequent model predictions. Overparameterization may also mask systematic errors in the conceptual model. To alleviate the difficulties caused by an ill-posed inverse problem, it may be appropriate to include prior information about the parameters or to apply regularization methods.

Different options are available in iTOUGH2 to parameterize heterogeneity, providing the means to identify hydrogeologic structures and to examine their impact on inverse modeling results and/or model predictions.

MODELING HETEROGENEITY IN iTOUGH2

In the standard zonation approach, constant properties are assigned to groups of elements of the discretized model. This representation of (usually large-scale) heterogeneity requires prior knowledge about the geometry of hydrogeologic units. If stratigraphic information is available, the number of parameters to be estimated can be sufficiently reduced, often yielding a well-posed inverse problem. However, if the subsurface structure is essentially random on the scale of interest, zonation may lead to a calibrated model that does not match the data well, or the estimated parameters are biased because of systematic errors in the model structure.

Subsurface heterogeneities often exhibit a hierarchical structure described by fractal distributions. These fractal hydrogeologic property distributions can be created using a set of affine transformations and an associated set of probabilities, which determine a so-called Iterated Function System (IFS). Each IFS has a unique attractor, which can be described by a relatively small number of parameters. Following the procedure outlined in Doughty (1995), iTOUGH2 generates fractal sets, which are subsequently mapped to hydrogeologic properties (see Figure 1). This method is flexible enough to create fractals with linear, areal, and volumetric structures. Solving the related inverse problem often requires the use of a robust, albeit relatively inefficient search method (such as Simulated Annealing).

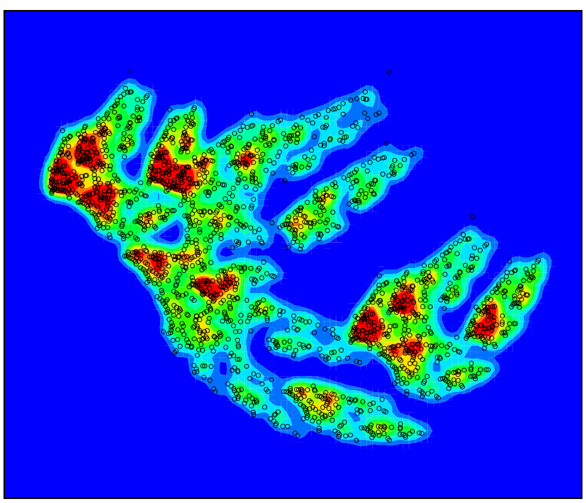

Figure 1. Fractal permeability field, created from IFS-generated attractor points (open circles).

Geostatistical methods are widely used to characterize heterogeneity and to generate realizations of spatially variable property fields. A number of interpolation methods (such as kriging; see Figure 2a) and simulation techniques (such as sequential Gaussian simulation (see Figures 2b and 2c) and sequential indicator simulation) have been incorporated into iTOUGH2 based on the codes provided by the Geostatistical Software Library GSLIB (Deutsch and Journel, 1992). Internal generation of the heterogeneous property field and its mapping onto the numerical grid makes geostatistical parameters accessible to estimation by inverse modeling. This means that geostatistical parameters (such as the correlation length) are automatically adjusted to directly match pressure and concentration data, rather than to adapt to an empirical variogram.

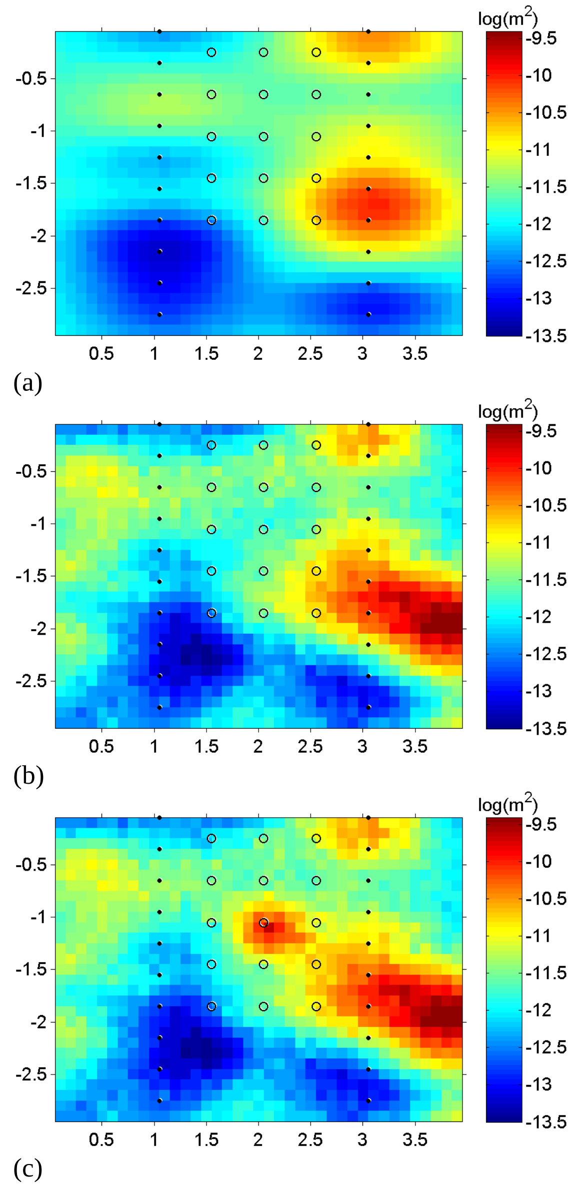

Figure 2. Spatially correlated permeability field created by kriging (a), and sequential Gaussian simulation (b and c). The fields are conditioned on permeability data along two vertical boreholes (black dots). Open circles indicate pilot points. Changing the permeability at the center pilot point affects the field in its immediate vicinity (compare (b) and (c)).

The geostatistically generated property fields can be conditioned on given values at certain locations. While conditioning is usually invoked to honor measured values, it also can be used to adapt so-called pilot points (RamaRao et al., 1995) or master points (Gómez-Hernández et al., 1997). In this approach, property values at the pilot points are the parameters of calibration. This approach couples geostatistics and optimization. As shown in Figures 2b and 2c, changing the permeability at one of the pilot points influences the permeability field in the vicinity of the point within approximately one correlation length. Distributing pilot points over the model domain allows iTOUGH2 to modify the heterogeneous field during an inversion, improving the match to the measured data of the system response, and at the same time acknowledging the geostatistical properties of the field as well as measured permeabilities. An application of the pilot point method using iTOUGH2 is presented in Kowalsky et al. (2003).

APPLICATIONS

The following examples illustrate some iTOUGH2 applications, in which the model structure (specifically heterogeneity) is examined either through the estimation of effective parameters or through sensitivity and uncertainty propagation analyses.

Seepage into Underground Opening

Dripping of water into tunnels containing nuclear wastes is a key mechanism affecting the concentration and rate at which dissolved radionuclides migrate away from the repository. In unsaturated formations, water tends to flow around the opening on account of the capillary-barrier effect, preventing seepage from occurring or reducing seepage flux below the prevalent percolation flux.

While the capillary-barrier effect is well understood for underground openings in homogeneous formations or layers of uniform porous media, numerical modeling is required to study seepage from fractured rock such as welded tuffs. Fractured rock can be considered a highly heterogeneous medium, where fractures are connected regions of high permeability and low capillarity, interspersed with matrix blocks of low permeability and high capillarity. The location, size, and orientation of fractures as well as the hydraulic properties within rough-walled fracture planes tend to be random. The random nature is built into discrete fracture network models, which generate realizations of fracture sets based on their statistical characteristics. An example of this approach is presented by Liu et al. (2002), who generated a two-dimensional TOUGH2 model of discrete fractures (Figure 3) and simulated flow and seepage into a circular opening (Figure 4).

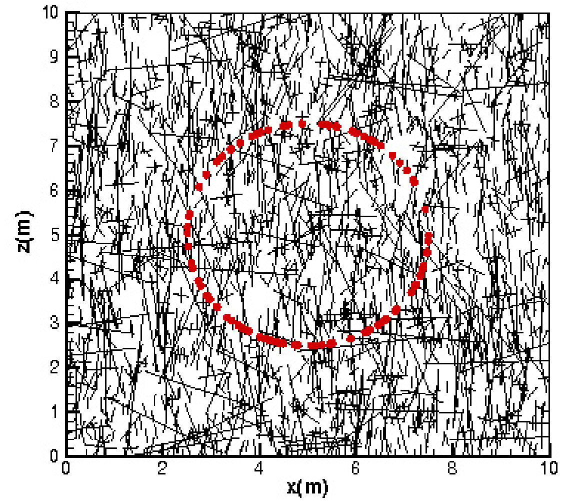

Figure 3. Discrete fracture network model for TOUGH2 (after Liu et al., 2002).

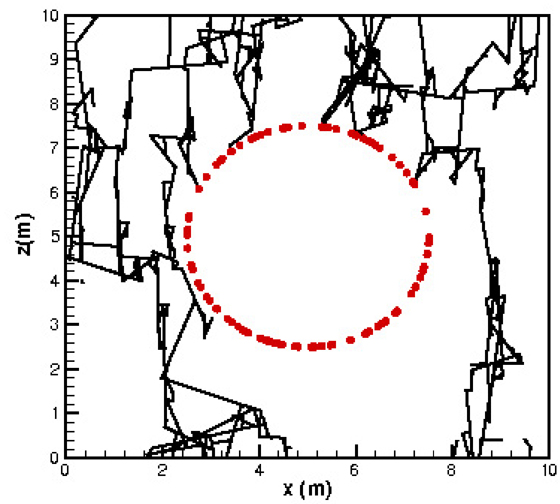

Figure 4. Flow paths through discrete fracture network inducing seepage into underground opening (after Liu et al., 2002).

The development of a site-specific discrete fracture network model requires collecting a large amount of geometric and hydrologic data. While part of the geometric information can be obtained from fracture mappings, the description of the network remains incomplete and potentially biased towards fractures of a certain orientation and a certain size. Moreover, unsaturated hydrological parameters on the scale of individual fractures are required, along with conceptual models and simplifying assumptions regarding unsaturated flow within fractures and across fracture intersections. Because these databases are often not available and generally difficult or even impossible to obtain for site-specific simulations, such a model must be calibrated against hydrogeologic data, such as seepage rates collected during a liquid-release test.

A calibrated heterogeneous fracture continuum model is a viable alternative to the discrete fracture network model described above. Because fractures are not perfectly parallel to the tunnel axis (which is an implicit assumption of 2D discrete fracture network models), water can be diverted around the opening also *within* the fracture plane, leading to a less discrete system behavior. Moreover, accepting the fact that parameters used in a numerical model are always (1) related to the conceptual model and its numerical implementation, (2) specific to the involved physical processes, (3) dependent on the scale, and (4) tailored to the prediction variables of interest, the calibration of the model against relevant data yields effective continuum parameters that are not only appropriate, but optimal for the given model and study objectives. This overall approach has been examined for the seepage problem discussed above.

Finsterle (2000b) demonstrated that seepage into underground openings excavated from a fractured formation could be simulated using a heterogeneous fracture continuum model, provided that the model is calibrated against seepage-relevant data (such as data from liquid-release tests). A two-dimensional high-resolution model was created with multiple sets of elongated features representing heterogeneous fractures, which are embedded in a low-permeability matrix (Figure 5). An excavation-disturbed zone was introduced by increasing permeability around the opening This model is capable of creating discrete flow and seepage behavior (see Figure 6), and is thus referred to as a discrete-feature model. Synthetically generated seepage data from a liquid-release test simulated with this discrete-feature model were used to calibrate a simplified heterogeneous fracture continuum model.

The calibrated continuum model was then used to predict seepage rates into a sufficiently large section of an underground opening for low percolation fluxes, i.e., conditions significantly different from those encountered during calibration. Monte Carlo simulations were performed to examine prediction uncertainty as a result of uncertainties in the input parameters. Moreover, a new realization of the underlying heterogeneous permeability field was generated for each realization, capturing the impact of variability that can only be characterized stochastically.

As shown in Figure 7, prediction uncertainty is substantial, mainly because of the strong impact of local heterogeneity on seepage, which cannot be described deterministically. Nevertheless, the seepage percentages predicted with the continuum model are consistent with the synthetically generated data from the discrete-feature model. This demonstrates that (1) the calibrated continuum model and discrete-feature model yield consistent estimates of the seepage threshold and average seepage rates, and (2) that the continuum approach is appropriate for performing seepage predictions even if extrapolated to percolation fluxes that are significantly lower than those induced by liquid-release tests, which were performed at relatively high injection rates to generate seepage data useable for model calibration.

The general modeling approach examined by inverting and predicting synthetic data has been successfully applied to the analysis of seepage-rate data from actual liquid-release tests. These iTOUGH2 analyses are discussed in Ghezzehei et al. (2003).

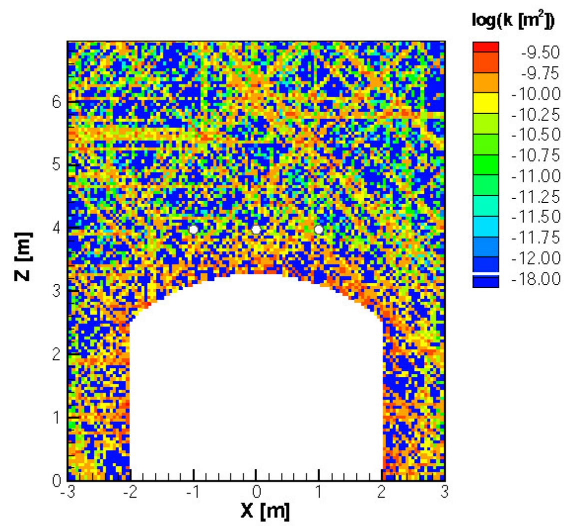

Figure 5. Discrete-feature model for TOUGH2 (after Finsterle, 2000b).

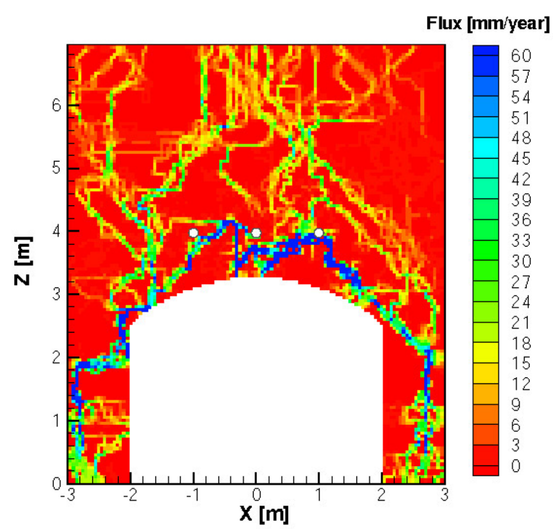

Figure 6. Flow through discrete fracture network and seepage into underground opening (after Finsterle, 2000b).

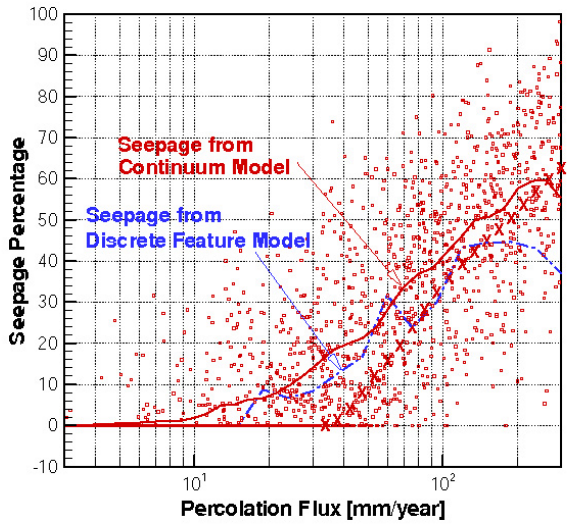

Figure 7. Seepage prediction with calibrated fracture continuum model (solid line) including results from Monte Carlo simulations (dots) and comparison to synthetic seepage data provided by the discrete-feature model (dash-dotted line). Crosses indicate the simulations with the calibrated parameter set and the permeability realization used during the inversion (after Finsterle, 2000b).

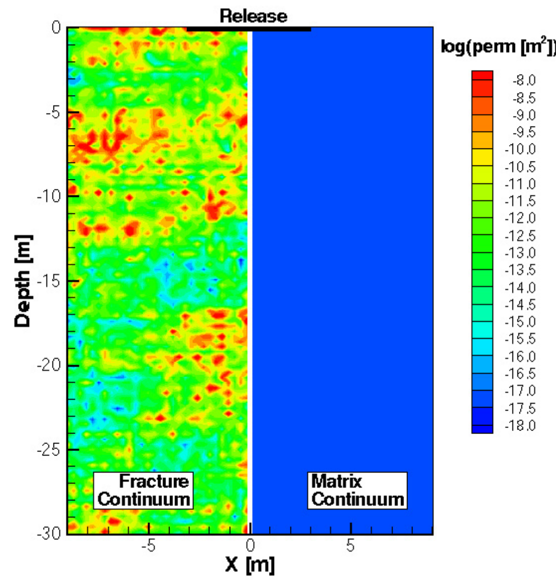

Figure 8. One realization of the heterogeneous permeability field for the fracture continuum; the matrix is homogeneous. The model is symmetric about the line X = 0. While both the fracture and matrix continua occupy the entire model domain, the fracture continuum is shown on the left and the matrix on the right of the symmetry axis.

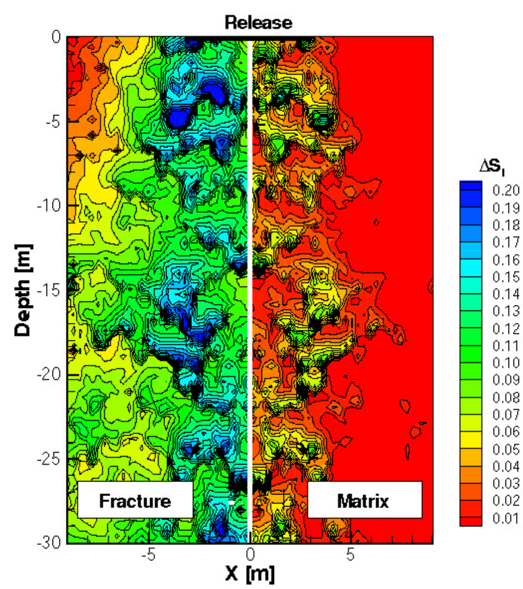

Figure 9. Saturation changes induced by release of a water pulse at |X| < 3 for one day. The model is symmetric about the line X = 0. While both the fracture and matrix continua occupy the entire model domain, the fracture continuum is shown on the left and the matrix on the right of the symmetry axis.

Migration of Water Pulse in Fractured Rock

Contaminant transport is strongly affected by the presence of fractures and the degree of fracture-matrix interaction. Measurements of chemical signatures at fractured sites often represent matrix concentrations—contaminated water may penetrate much deeper and faster through the fracture network. It is therefore crucial to understand and accurately model the process of matrix imbibition, which is affected not only by the sorptivity of the matrix, but also by the characteristics of the fractures.

iTOUGH2 simulations of water flow through fractured rock were performed to examine the penetration depth of a large pulse of water entering such a system. The influences of local heterogeneities in the fracture network and variations in hydrogeologic parameters were examined by sensitivity analyses and Monte Carlo simulations. To resolve the pressure and saturation gradients between the fractures and the matrix, the method of "Multiple Interacting Continua" (MINC; Pruess and Narasimhan, 1982, 1985) was employed. A two-dimensional heterogeneous fracture permeability field was generated, exhibiting both local obstacles in the fracture continuum as well as high-permeability channels (Figure 8). These obstacles may represent dead-end fractures, discontinuities in the fracture network, asperity contacts, or heterogeneity in the amount and properties of fracture fillings. The matrix is assumed homogeneous.

A pulse of water was uniformly applied for one day at the top of the model for |X| < 3 m. As shown in Figure 9, heterogeneity in the fracture continuum leads to an intricate distribution of saturation changes, which is subsequently imprinted on the matrix despite its homogeneity. The saturation changes in the matrix give an indication of the strength of matrix imbibition, which is affected by the residence times of water in the adjacent fractures and the matrix sorptivity properties. Once water enters the matrix, it remains essentially stagnant, because the relatively strong capillarity prevents water from flowing back into the fractures after the pulse has passed. The saturation changes disperse gradually (driven by capillary pressure gradients), and slowly migrate downwards in accordance with the low matrix permeability. Consequently, these signals remain visible for a long time. On the other hand, the perturbation dissipates quickly in the fracture continuum because of its high permeability.

If the saturation changes are caused by imbibition of contaminated water, they may induce matrix contaminant concentrations that are higher than background values. The simulated saturation-change in the matrix distribution of Figure 9 is qualitatively consistent with observed contaminant profiles, which typically show sections of apparently uncontaminated rock interrupted by spikes with high concentration values. Since water that quickly flows through the fracture network may not leave a prominent chemical signal in the matrix, the apparent absence of elevated contaminant concentrations at certain measurement locations along a vertical profile does not necessarily indicate the actual penetration depth of the contamination, which may be much greater.

A detailed sensitivity analysis of contamination signals in a fractured porous medium can be found in Finsterle et al. (2002).

CONCLUDING REMARKS

iTOUGH2 can be used to support a variety of scientific studies and engineering tasks, including test design, sensitivity analyses, parameter estimation, uncertainty propagation analyses, and testing of alternative conceptual models. The main advantage of iTOUGH2 as an optimization tool is the fact that it is based on the TOUGH2 simulator. This ensures that complex subsurface flow and transport processes are accurately represented. However, despite its physical basis, it should be recognized that modeling always involves a sequence of steps in which the physical system is simplified and reduced to its salient features. As a result of this abstraction process, it is necessary to determine and use effective parameters that are related to the specific conceptual model. This limits the applicability of the model and the generality of its parameters. On the other hand, the estimation of effective parameters by calibrating the model against suitable data of good quality leads to site-specific, model-related, and process-relevant parameters that can be considered optimal for the given modeling task.

Changes in the conceptual model usually have the greatest impact on model predictions and thus on the conclusions of a study. The following iTOUGH2 features support the evaluation of alternative conceptual models:

- *Automatic Model Calibration*: The process of matching the model output to observed data by adjusting sensitive parameters helps determine whether or not the conceptual model is a likely representation of the natural system. Moreover, automatic calibration allows for a quick evaluation of multiple alternative models.

- *Residual and Error Analyses*: A statistical analysis of the discrepancies between the calculated and observed system response points towards aspects of the conceptual model that may need to be refined. The error analysis of the estimated parameters may indicate that the problem is overparameterized.

- *Parameterization*: The flexible architecture of iTOUGH2 allows a user to parameterize certain aspects of the conceptual model, and thus be able to submit them to a formalized analysis and optimization. For example, geostatistical tools can be used to describe complex heterogeneity with just a few parameters, which can then be estimated or perturbed in a sensitivity analysis. Similarly, suspected modeling errors or artifacts and trends in the data can also be parameterized.

- *Monte Carlo Simulations*: Monte Carlo simulations conducted with iTOUGH2 evaluate the prediction uncertainty as a result of uncertainty in the input parameters. (Note that statistical correlations among the parameters can be taken into account.) Consequently, the impact of *parameterized* aspects of the conceptual model can also be examined. Moreover, for each Monte Carlo simulation, a new realization of the stochastic property field can be generated to examine variability as a result of unspecified randomness.

- *Model Identification Criteria*: iTOUGH2 calculates a number of model identification criteria, which allow comparing models with different numbers of adjustable parameters.

- *Test Design*: iTOUGH2 can be used to perform synthetic inversions in support of experimental design. The calculated measures regarding the information content of potential measurements and the correlation structure of the parameters to be estimated indicate whether a proposed design is capable of distinguishing between competing theories or conceptual models.

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http://www-esd.lbl.gov/iTOUGH2

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